William E. Acree, Jr. and James S. Chickos

The thermochemical behavior of more than 3000 organic compounds known to form liquid crystals is reported along with references to the original literature. A group additivity approach used to estimate total phase change entropies of organic molecules applied to 627 of these liquid crystals is found to significantly over-estimate their total phase change entropies. Comparison of experimental and estimated values also show significant scatter relative to database compounds. The origins of these discrepancies are discussed in terms of a model used to explain liquid crystal formation.

L. Zarkova, U. Hohm, and M. Damyanova

Reference tables of second pVT-virial coefficients $B(T)$, viscosity $\eta(T)$, and self-diffusion $\rho D(T)$ are given for all neat alkanes C_nH_{2n+2}, $n<6$, for temperatures $T \leq 1200$ K. By restricting ourselves to low densities, the thermophysical properties are calculated by means of an isotropic (n-6) Lennard-Jones temperature-dependent potential.

Xuehua Li, Jingwen Chen, Li Zhang, Xianliang Qiao, and Liping Huang

The octanol-air partition coefficient (K_{OA}) is a key physicochemical parameter for describing the partition of organic pollutants between air and environmental organic phases. In the present study, a fragment constant model based on five fragment constants and one structural correction factor, was developed for predicting log K_{OA} at temperatures ranging from 10 to 40 °C. The model was validated as successful by statistical analysis and external experimental log K_{OA} data. As aromatic compounds that contain C, H, O, Cl, and Br atoms, were included in the training set used to develop the model, the current fragment model applies to a wide range of chlorinated and brominated aromatic pollutants.

Qingfeng Zeng, Kehe Su, Litong Zhang, Yongdong Xu, Laifei Cheng, and Xiutian Yan

CH_3SiCl_3 (methyltrichlorosilane) (MTS) is one of the most important precursors for manufacturing both an oxidation resistant SiC coating and a functional SiC flim by chemical vapor deposition (CVD). In order to analyze the decomposition products of MTS with a thermodynamic calculation, correct thermodynamic data must be obtained from the authoritative data sources. G3(MP2) has been applied to evaluate the thermodynamic data of MTS(gas). The calculated value of the Gibbs energy of formation, $\Delta_f G_m^0(298.15 \text{ K}) = -490.13$ kJ·mol^{-1}, compares with a value, $\Delta_f G_m^0(298.15 \text{ K}) = -468.02$ kJ·mol^{-1} from the 4th edition of the NIST-JANAF Thermochemical Tables. Further analyses have been conducted: (1) by using G3, G3//B3LYP and G3(MP2)//B3LYP theories, (2) by using variable scale factors for G3(MP2) theory, and (3) by investigating the accuracy of both experimental and calculated thermodynamic data. The calculated values can provide $\Delta_f G_m^0$ values for MTS above 1500 K. The final fitted equation for MTS(gas) is: $\Delta_f G_m^0 = 7.5763 \times 10^{-6} T^2 + 1.9649 \times 10^{-1} T - 5.4817 \times 10^2$, where T is absolute temperature.

Marian Góral, Barbara Wiśniewska-Gocłowska, and Andrzej Mączyński

The recommended liquid–liquid equilibrium (LLE) data for 19 binary 1-alkanol–water systems have been obtained after critical evaluation of all data (527 data sets) reported in the open literature up to the end of 2004. An equation for prediction of the 1-alkanol solubility was developed. The predicted 1-alkanol solubility was used for calculation of water solubility in the second liquid phase. The LLE calculations were done with the equation of state appended with a chemical term proposed by Góral.

G. Scalabrin, P. Marchi, and R. Span

A multiparameter viscosity equation for propane, valid in wide temperature and pressure ranges, was developed through an optimization technique for the functional form. This is a significant improvement with respect to the reference equation available in the literature. Both the development and the evaluation of the viscosity equation requires a highly accurate equation of state in order to convert the independent variables used for the experimental data, in most applications (T,P), into the independent variables of the viscosity equation (T,ρ).

Anna Salmon and Didier Dalmazzone

A predictive method, based on Benson's group additivity technique, was developed for calculating the enthalpy of formation in the solid phase, at 298.15 K, of carbon-hydrogen compounds and carbon-hydrogen-oxygen compounds. A complete database compiles 398 experimental enthalpies of formation.